REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	Dec. 1995	FINAL, 31 July 94 - 31 July 96

4. TITLE AND SUBTITLE
Thermal Stresses in Thin Films and Interconnects

5. FUNDING NUMBERS
G#F49620-94-1-0290

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AFOSR-TR-97

0280

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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
AFOSR
110 Duncan Avenue
Bolling AFB, Washington D.C. 20332-0001

NA

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES
The computational portion of the report to be also published in *Computers and Structures* (Spring 1997)

12a. DISTRIBUTION / AVAILABILITY STATEMENT
Unlimited

12b. DISTRIBUTION CODE

DISTRIBUTION STATEMENT A
Approved for public release;
Distribution Unlimited

19970616 137

13. ABSTRACT (Maximum 200 words)

The two-dimensional closed system of partial differential equations and boundary conditions were derived with respect to thermal stresses in thin films and bonding layers of electronics for an arbitrary shape of a film/layer in plan view.

Both thermoelastic materials with arbitrary temperature-dependent constants and ideally-thermoplastic materials were studied. Analytical solutions based on boundary layer philosophy were constructed, and the numerical code for thermal stresses in thin films and bonding layers was suggested.

DTIC QUALITY INSPECTED 3

14. SUBJECT TERMS	15. NUMBER OF PAGES
Thin films; Bonding layers; Analytical theory; Thermal stresses; Ceramics; Metals	55
	16. PRICE CODE: $43,648

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
Unclassified	Unclassified	Unclassified	UL

Final Technical Report

Grant No. F49620-94-1-0290 for $43,648.00

From August 1, 1994 to July 31, 1996

RESIDUAL AND THERMAL STRESSES IN THIN FILMS AND INTERCONNECTS

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Abstract

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ABSTRACT

1. OBJECTIVES

The original objective for the study was the construction of analytical theory for thermal/residual stresses in thin films and bonding layers. However, prompted by the reviewers of the *Journal of Applied Physics,* the P.I. involved one more goal, namely the construction of numerical codes for the 2D and 3D fields, which caused the prolongation of the planned work to the second year.

2. STATE-OF-THE-ART IN THE FIELD BEFORE AND AFTER THE WORK IS DONE

Thermal/residual stresses in thin films and bonding layers are currently the main problem of reliability in high speed electronics. Only simple 1D problems or heavy numerical experiments overloaded by unnecessary information were available in literature before. The work was proposed to derive the closed system of partial differential equations with respect to thermal stresses, which would take into account the main simplifying feature of the problem, namely the small thickness of films and bonding layers compared to their dimensions in plan view. To this end, the approach taken from the dynamics of viscous fluids and pioneered by Prandtl was used. As a result, such systems and necessary boundary conditions were derived, providing the 2D analytical theories for thermal elastic stresses in thin surface films and thin bonding layers. An analogous study was performed for total plastic deformation of thin films and bonding layers, and the closed equation system of the theory of plasticity was derived for both.

A finite difference numerical code based on the analytical theory was developed and verified in some calculations.

3. ACCOMPLISHMENTS

For the first time, the 2D analytical theory of thermal/residual stresses in thin films and bonding layers was derived. This achievement is similar to the construction of the theory of plates and shells by Kirchhoff and Love a century ago. The system of partial differential equations appeared to have a specific structure with small parameters before the senior derivatives, which is characteristic for boundary layer problems, and preliminary numerical experiments unveiled a boundary layer near the trim of a thin film and/or bonding layer in plan view.

4. PERSONNEL

Luiz Martinez took part in the numerical calculations of thermal stresses in thin films without a financial support from this grant.

5. PUBLICATIONS

1. On the theory of thermal stresses in a thin film on a ceramic substrate, *J. Appl. Phys.*, 75(2), pp. 844-849, 1994.

2. On the theory of thermal stresses in a thin bonding layer, *J. Appl. Phys.*,**78**(11), pp. 6826-6832, 1995.

3. A computerized model for thermal stresses in thin films, *Computers and Structures* (jointly with L. Martinez), to be published in Spring 1997.

4. Flow past a cylinder of an arbitrary cross section in a saturated porous medium under any Peclet number, *SIAM J. on Applied Mathematics*, (to be published in Spring 1997). One section in this paper treats an application of the derived solution to the growth of planar voids in fine lines described by the 2D diffusion-electromigration of vacancies in the field of tensile stresses and temperature.

6. NEW DISCOVERIES AND INVENTIONS

New effects of Poisson's ratio mismatch and periodic law of thermal stress distribution in plastic region were discovered.

No inventions or patent disclosures were performed.

PART 1
THE THEORY OF THERMAL STRESSES IN THIN FILMS

It is generally recognized that thermal stresses in thin films are primarily responsible for morphological changes in thin films, including hillocks, whiskers, and void or pit formations, which present serious problems of reliability in microelectronics. In Part I, the analytical theory of thermal stresses is constructed under some natural simplifying assumptions. The latter include that of the thermoelastic or thermoelastic-plastic behavior of the materials of a film and substrate after depositing the film and cooling the composite system to an operational temperature. The closed system of governing partial differential equations for thermal stresses in a thin film is derived for any in-plane shape of the film. Some particular problems are solved in an explicit form and the implication of the solutions for the prediction of hillocks is discussed.

1. INTRODUCTION

Suppose, for example[1], that Pb is deposited on a Si substrate at room temperature in the form of a thin film, and then the composite material is cooled to 4.2 K where the Pb becomes superconducting. The coefficients of the thermal expansion of Pb and Si are $29.5\times10^{-6}/°C$ and $2.6\times10^{-6}/°C$, respectively. While the Pb tries to shrink, the Si substrate restricts it from doing so; hence, in cooling, the Pb is under tension. These thermal stresses may include plastic yielding of the film and the formation of hillocks.[2-4] An analogous phenomenon is possible for some semiconducting alloys deposited on a substrate and cooled to the nitrogen temperature where some semiconductors become superconductive. Upon heating the composite back to room temperature, the thin film tends to expand and again is restricted by the substrate. Thus, the thin film is under compression upon heating.

In Part I, the analytical theory of thermal stresses in thin films is constructed subject to the following assumptions:

1. The thickness of a film is much smaller than the thickness of a substrate and any in-plane dimension of the film and substrate.
2. No shear or open-mode cracks are formed during the deformation process by cooling/heating (ideal bonding).
3. The material of the substrate is homogeneous, isotropic, and linearly thermoelastic.
4. The material of the film is homogeneous, isotropic, and ideally thermoelastic-plastic.

This treatment is based on ideas advanced earlier as applied to simiplier problems[5].

2. SYSTEM OF GOVERNING EQUATIONS

A. Thin film

Consider a thin film deposited on a substrate (Fig. 1). For clarity, the film is depicted in Fig. 1 in plan view in a rectangular form having dimensions of $2l_x \times 2l_y$. However, the theory treated below is valid for any film form. The plane, z=0, is chosen along the flat film-substrate interface and a possible film-unprotected surface of the substrate. The planes, y=0 and x=0, coincide with the planes of symmetry. It is assumed that the boundary surface of the thin film at z=t is free of tractions (t is the film thickness):

$$\text{when} \quad z = t, \; |x| < l_x, \quad |y| < l_y \quad \sigma_z = \tau_{zx} = \tau_{zt} = 0. \tag{2.1}$$

The edges of the film are also free of tractions:

$$\text{when} \quad \begin{array}{ll} 0<z<t\ x=\pm l_x & \sigma_x=\tau_{xy}=\tau_{xz}=0; \\ 0<z<t\ y=\pm l_y & \sigma_y=\tau_{xy}=\tau_{yz}=0. \end{array} \tag{2.2}$$

The film-substrate interface at z=0 is ideally bonded so that all displacements and stresses, σ_z, τ_{zx}, and τ_{zy}, are continuous across the interface. Designate that

$$\tau_x=\tau_{zx}\ at\ z=0; \quad \tau_y=\tau_{zy}\ at\ z=0 \tag{2.3}$$

In what follows, the stress, σ_z, is considered negligibly small in both the thin film and substrate boundary zone influenced by the thin film and located near the latter. Therefore, the equilibrium equation with respect to the z axis is not essential and can be omitted.

Consider the equilibrium equations with respect to the x and y axes:

$$\frac{\partial\sigma_x}{\partial x}+\frac{\partial\tau_{xy}}{\partial y}+\frac{\partial\tau_{zx}}{\partial z}=0, \tag{2.4}$$

$$\frac{\partial\sigma_y}{\partial y}+\frac{\partial\tau_{xy}}{\partial x}+\frac{\partial\tau_{yz}}{\partial z}=0. \tag{2.5}$$

Here, σ_x, σ_y, τ_{xy}, τ_{zx}, and τ_{yz} are stresses.

Let us integrate Eqs. (2.4) and (2.5) over z from z=0 to z=t. Using Eqs. (2.1) and (2.3) we derive

$$\frac{\partial\bar{\sigma}_x}{\partial x}+\frac{\partial\bar{\tau}_{xy}}{\partial y}=\frac{\tau_x}{t}, \tag{2.6}$$

$$\frac{\partial\bar{\sigma}_y}{\partial y}+\frac{\partial\bar{\tau}_{xy}}{\partial x}=\frac{\tau_y}{t}. \tag{2.7}$$

Here, $\bar{\sigma}_x(x,y), \bar{\sigma}_y(x,y)$, and $\bar{\tau}_{xy}(x,y)$ are corresponding mean stresses in a thin film:

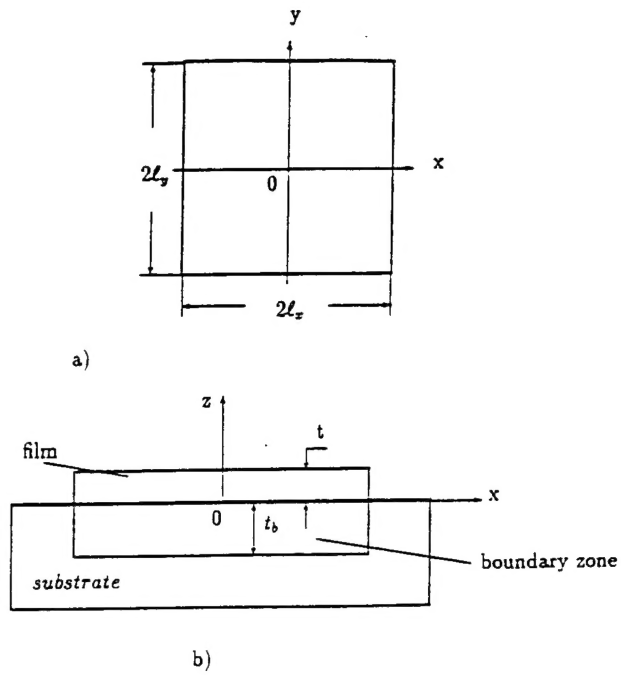

FIG. 1. Schematic representation of a film-substrate composite: (a) planar view of a deposited thin film, with dimensions, $2l_x \times 2l_y \times t$. (b) Sectional view showing the substrate boundary zone with dimensions $2l_x \times 2l_y \times t_b$.

$$\overline{\sigma}_x = \frac{1}{t}\int_0^t \sigma_x \, dz, \quad \overline{\sigma}_y = \frac{1}{t}\int_0^1 \sigma_y \, dz, \quad \overline{\tau}_{xy} = \frac{1}{t}\int_0^t \tau_{xy} dz. \tag{2.8}$$

Prior to when yielding occurs, the film material is thermoelastic and satisfies the following incremental Hooke's law equations:

$$\frac{\partial(\Delta U)}{\partial x} = \frac{\Delta\overline{\sigma}_x - \upsilon_f \Delta\overline{\sigma}_y}{E_f} + \alpha_f \Delta T, \tag{2.9}$$

$$\frac{\partial(\Delta V)}{\partial y} = \frac{\Delta\overline{\sigma}_y - \upsilon_f \Delta\overline{\sigma}_x}{E_f} + \alpha_f \Delta T, \tag{2.10}$$

$$\frac{\partial(\Delta V)}{\partial y} + \frac{\partial(\Delta V)}{\partial x} = \frac{\Delta\tau_{xy}}{G_f}. \tag{2.11}$$

Here, U(x,y) and V(x,y) are mean displacement components along the x and y axes, respectively (in a thin film), E is Young's modulus, G is the shear modulus, ν is Poisson's ratio, and α is the thermal expansion coefficient. Subscript f corresponds to the film material. The value of T denotes the temperature with respect to a certain reference temperature when all thermal stresses equal zero. (In the example of the Introduction, the reference temperature is room temperature, at which Pb is deposited on Si.) The symbol Δ designates the infinitesimal increment of a quantity in the thermal process of heating or cooling corresponding to the growth ΔT of the temperature. The parameters α, E, G, and ν, generally, are some functions of temperature. Equations (2.6) and (2.7) hold for stress increments, too.

B. Substrate

A thin film influences the stress and strain field of a substrate in a certain boundary zone in the neighborhood of the thin film. Outside the boundary zone, the stress and strain field is not perturbed by a thin film, hence it is the same field as without the thin film. We assume that the boundary zone occupies the domain $0 > z > - t_b$, $|x| < l_x$ and $|y| < l_y$, in Fig. 1(b), where t_b is the thickness of the boundary zone. The value of t_b , if unknown from the physical formulation of a problem, is considered as a fitting parameter, which can be chosen to better approximate the function of primary interest. For example, in the case of a rigid, strip-shaped thin film, it was determined that[5] from a comparison with the exact solution, t_b roughly equals one-sixth of the strip width.

Due to bonding with no slipping between a thin film and substrate, and because of the small thickness of the thin film, we can ignore the bending stresses in the film. Under these

conditions, the thin film can induce in substrate only shear stresses, τ_{xz} and τ_{yz}, and in-plane displacements, u and v, and in-plane stresses, σ_x, σ_y, and τ_{xy}. Equilibrium equations with respect to the x and y axes have the form of Eqs. (2.4) and (2.5). In the substrate boundary zone, we have

$$\frac{\partial}{\partial z} >> \frac{\partial}{\partial x} \quad \text{and} \quad \frac{\partial}{\partial z} >> \frac{\partial}{\partial y} \quad ,$$

so that Eqs. (2.4) and (2.5) take the following form:

$$\frac{\partial \tau_{xz}}{\partial z} = 0 \quad , \qquad \frac{\partial \tau_{yz}}{\partial z} = 0 \qquad (2.12)$$

Also, in the boundary zone we have

$$\frac{\partial u}{\partial z} >> \frac{\partial w}{\partial x} \quad , \qquad \frac{\partial v}{\partial z} >> \frac{\partial w}{\partial y}$$

where u, v, and w are displacement components, so that the incremental Hooke's law can be written in the form

$$\frac{\partial(\Delta u)}{\partial z} = \frac{\Delta\tau_{xz}}{G_s} \quad , \qquad \frac{\partial(\Delta v)}{\partial z} = \frac{\Delta\tau_{yz}}{G_s} \quad . \qquad (2.13)$$

Subscript s corresponds to the substrate material. The Δ is an infinitesimal increment of a quantity in the heating-cooling process corresponding to the growth, ΔT, of the temperature.

Integrating Eqs. (2.12) and (2.13) over z, we obtain

$$\tau_{xz} = \tau_x(x,y) \quad , \qquad \tau_{yz} = \tau_y(x,y) \quad , \qquad (2.14)$$

$$\Delta u = z\frac{\Delta\tau_x}{G_s} + \Delta U(x,y) \quad , \qquad \Delta v = z\frac{\Delta\tau_y}{G_s} + \Delta V(x,y) \quad . \qquad (2.15)$$

Here, we used the equilibrium and continuity equations on the film-substrate interface. Moreover, the following compatibility equations should be satisfied:

$$\text{when} \quad z = t_b \qquad \Delta u = \Delta u_0 \ , \quad \Delta v = \Delta v_0 \ . \tag{2.16}$$

Here, u_0 (x,y) and v_0 (x,y) are the corresponding displacements, u and v, of the field unperturbed by the film. The functions u_0 and v_0 should be determined from analysis of the internal stress and strain field in a substrate without a film. In the following, they are considered given. For example, if the substrate without a film suffers an unconstrained uniform thermal deformation, we have

$$\text{when} \quad z = -t_b \ : \quad \Delta u_0 = x\alpha_s \Delta T \ , \qquad \Delta v_0 = y\alpha_s \Delta T \ . \tag{2.17}$$

[Here, we also used the symmetry condition in Fig. 1.(a).]

Thus, from Eqs. (2.15) and (2.16), it follows that

$$\Delta U = \Delta u_0 + \frac{t_b \Delta\tau_x}{G_s} \ , \tag{2.18}$$

$$\Delta V = \Delta v_0 + \frac{t_b \Delta\tau_y}{G_s} \ , \tag{2.19}$$

Substituting ΔU and ΔV in Eqs. (2.9), (2.10), and (2.11) by Eqs. (2.18) and (2.19), we obtain

$$\frac{\Delta\bar{\sigma}_x - v_f \Delta\bar{\sigma}_y}{E_f} = \frac{t_b}{G_s}\frac{\partial(\Delta\tau_x)}{\partial x} + \frac{\partial(\Delta u_0)}{\partial x} - \alpha_f \Delta T \ , \tag{2.20}$$

$$\frac{\Delta\bar{\sigma}_y - v_f \Delta\bar{\sigma}_x}{E_f} = \frac{t_b}{G_s}\frac{\partial(\Delta\tau_y)}{\partial y} + \frac{\partial(\Delta v_0)}{\partial y} - \alpha_f \Delta T \ , \tag{2.21}$$

$$\frac{\Delta\bar{\tau}_{xy}}{G_f} = \frac{t_b}{G_f}\left(\frac{\partial(\Delta\tau_x)}{\partial y} + \frac{\partial(\Delta\tau_y)}{\partial x}\right) + \frac{\partial(\Delta u_0)}{\partial y} + \frac{\partial(\Delta v_0)}{\partial x} \ . \tag{2.22}$$

From Eqs. (2.6) and (2.7), it follows that

$$\frac{1}{t}\Delta\tau_x = \frac{\partial\left(\Delta\overline{\sigma}_x\right)}{\partial x} + \frac{\partial\left(\Delta\overline{\tau}_{xy}\right)}{\partial y} \quad , \tag{2.23}$$

$$\frac{1}{t}\Delta\tau_y = \frac{\partial\left(\Delta\overline{\tau}_{xy}\right)}{\partial x} + \frac{\partial\left(\Delta\overline{\sigma}_y\right)}{\partial y} \quad . \tag{2.24}$$

Substituting $\Delta\tau_x$ and $\Delta\tau_y$ in Eqs. (2.20)-(2.22) by Eqs. (2.23) and (2.24) provides

$$\begin{aligned}&\frac{\partial^2\left(\Delta\overline{\sigma}_x\right)}{\partial x^2} + \frac{\partial^2\left(\Delta\overline{\tau}_{xy}\right)}{\partial x\partial y}\\ &\quad = \frac{G_s}{tt_b}\left(\frac{\Delta\overline{\sigma}_x - \nu_f\Delta\overline{\sigma}_y}{E_f} - \frac{\partial\left(\Delta u_0\right)}{\partial x} + \alpha_f\Delta T\right) \quad ,\end{aligned} \tag{2.25}$$

$$\begin{aligned}&\frac{\partial^2\left(\Delta\overline{\sigma}_y\right)}{\partial y^2} + \frac{\partial^2\left(\Delta\overline{\tau}_{xy}\right)}{\partial x\partial y}\\ &\quad = \frac{G_s}{tt_b}\left(\frac{\Delta\overline{\sigma}_y - \nu_f\Delta\overline{\sigma}_x}{E_f} - \frac{\partial\left(\Delta v_0\right)}{\partial y} + \alpha_f\Delta T\right) \quad ,\end{aligned} \tag{2.26}$$

$$\begin{aligned}&\frac{\partial^2}{\partial x\partial y}\left(\Delta\overline{\sigma}_x + \Delta\overline{\sigma}_y\right) + \frac{\partial^2\left(\Delta\overline{\tau}_{xy}\right)}{\partial x^2} + \frac{\partial^2\left(\Delta\overline{\tau}_{xy}\right)}{\partial y^2}\\ &\quad = \frac{G_s}{tt_b}\left(\frac{\Delta\overline{\tau}_{xy}}{G_f} - \frac{\partial\left(\Delta u_0\right)}{\partial y}\right) \quad .\end{aligned} \tag{2.27}$$

The system of three partial differential equations, Eqs. (2.25)-(2.27), will serve to find the increments of thermal stresses $\overline{\sigma}_x$, $\overline{\sigma}_y$, and $\overline{\tau}_{xy}$ in a thin film in terms of *x* and *y*. In view of Eqs. (2.2) we have

$$
\begin{aligned}
&x = \pm l_x \qquad \Delta\bar{\sigma}_x = \Delta\bar{\tau}_{xy} = 0 \quad , \qquad \frac{\partial \Delta\bar{\sigma}_y}{\partial y} + \frac{\partial \Delta\bar{\tau}_{xy}}{\partial x} = 0 \quad , \\
&y = \pm l_y \qquad \Delta\bar{\sigma}_y = \Delta\bar{\tau}_{xy} = 0 \quad , \qquad \frac{\partial \Delta\bar{\sigma}_x}{\partial x} + \frac{\partial \Delta\bar{\tau}_{xy}}{\partial y} = 0 \quad .
\end{aligned}
\tag{2.28}
$$

The boundary value problem in Eqs. (2.25)-(2.28) is appropriate for both the analytical and numerical study of thermal stresses in thin films.

3. A STRIP-SHAPED THIN FILM ON A SUBSTRATE

Consider the case of Fig. 1(a) when $l_y >> l_x$, where a thin film is deposited in the form of an infinite strip, $|\,x\,| < l_x$, of width $2l_x$. In this case, due to the symmetry, we have

$$
\frac{\partial}{\partial y} = 0 \quad , \qquad \tau_{xy} = 0 \tag{3.1}
$$

We also assume that $\Delta u_0 = \alpha_s x \Delta T$ and $\Delta v_0 = \alpha_s y \Delta T$. With regard to Eq. (3.1), the governing equation system, Eqs. (2.25)-(2.27), become

$$
\frac{d^2\left(\Delta\bar{\sigma}_x\right)}{dx^2} = \frac{k^2}{l_x^2}\Delta\bar{\sigma}_x + F\Delta T \tag{3.2}
$$

Here,

$$
k^2 = \frac{l_x^2 G_s\left(1 - \nu_f^2\right)}{t t_b E_f} \quad , \tag{3.3}
$$

$$
F = \frac{G_s}{t t_b}\left(1 + \nu_f\right)\left(\alpha_f - \alpha_s\right) \quad , \tag{3.4}
$$

$$
\Delta\bar{\sigma}_y = \nu_f \Delta\bar{\sigma}_x - \left(\alpha_f - \alpha_s\right) E_f \Delta T \quad . \tag{3.5}
$$

The solution to Eq. (3.2) meeting the boundary condition, $\Delta\bar{\sigma}_x = 0$, when $x = \pm\, l_x$, is as follows:

$$\Delta\overline{\sigma}_x = F\Delta T \frac{l_x^2}{k^2} \left[\frac{\cosh\left(kx / l_x\right)}{\cosh k\,(T)} - 1 \right] dT \quad , \tag{3.6}$$

where F is a constant. It is just as easy to find the solution for the arbitrary function F = F (x). Since α_f, α_s, E_f, ν_f, and G_s are certain functions of temperature T, we integrate Eq. (3.6) over T and obtain

$$\begin{aligned} &\overline{\sigma}_x\,(T) - \overline{\sigma}_x\left(T_0\right) \\ &= l_x^2 \int_{T_0}^{T} \frac{F(T)}{k^2\,(T)} \left[\frac{\cosh\left(xk(T) / l_x\right)}{\cosh k\,(T)} - 1 \right] dT \end{aligned} \quad . \tag{3.7}$$

Here, T_o is the initial temperature of the heating/cooling process. Functions, F(T) and k(T) are defined by Eqs. (3.3) and (3.4), e.g., in the example problem of the Introduction, T_0 is the room temperature, T is the helium temperature, and

$$\overline{\sigma}_x\left(T_0\right) = 0 \quad , \tag{3.8}$$

and from Eq. (3.7), it follows that

$$\overline{\sigma}_x = l_x^2 \int_{T_0}^{T} \frac{F(T)}{k^2\,(T)} \left[\frac{\cosh\left(xk\,(T) / l_x\right)}{\cosh k\,(T)} - 1 \right] dT \quad , \tag{3.9}$$

$$\begin{aligned} \overline{\sigma}_y = &+ \int_{T_0}^{T} \left[\alpha_s\,(T) - \alpha_f\,(T)\right] E_f\,(T)\,dT \\ &+ l_x^2 \int_{T_0}^{T} \frac{\nu_f\,(T)F(T)}{k^2\,(T)} \left[\frac{\cosh\left(xk\,(T) / l_x\right)}{\cosh k\,(T)} - 1 \right] dT \end{aligned} \quad , \tag{3.10}$$

$$\overline{\tau}_x = t l_x \int_{T_0}^{T} \frac{F(T)\sinh\left(k\,(T)x / l_x\right)}{k^2\,(T)\cosh k\,(T)}\,dT \quad . \tag{3.11}$$

Thus, the thermal stresses are determined for arbitrary functions, α_f (T), α_s(T), E_f(T), G_s(T), and ν_f (T).

4. SOLUTION FOR LARGE k

The case of large k defined by Eq. (3.3) is of importance for very thin films, which is realized, for example, when $l_x^2 \gg tt_b$ and G_s is of the order of E_f. In this case, the solution to the governing equation system, Eqs. (2.25)-(2.27), constitutes a narrow boundary layer that borders the contour of a thin film. Everywhere inside the arbitrary contour of a film, except for the boundary layer, the solution is given by the following equations:

$$\Delta\bar{\sigma}_x - \nu_f \Delta\bar{\sigma}_y = E_f \Delta T \left(\frac{\partial}{\partial x} \frac{\Delta u_0}{\Delta T} - \alpha_f \right) \quad , \tag{4.1}$$

$$\Delta\bar{\sigma}_y - \nu_f \Delta\bar{\sigma}_x = E_f \Delta T \left(\frac{\partial}{\partial y} \frac{\Delta v_0}{\Delta T} - \alpha_f \right) \quad , \tag{4.2}$$

$$\Delta\bar{\tau}_{xy} = G_f \Delta T \left(\frac{\partial}{\partial x} \frac{\Delta v_0}{\Delta T} + \frac{\partial}{\partial y} \frac{\Delta u_0}{\Delta T} \right) \quad . \tag{4.3}$$

In a normal case, when $\Delta u_0 = \alpha_s x \Delta T$ and $\Delta v_0 = \alpha_s y \Delta T$, we have $\Delta\bar{\sigma}_x = \Delta\bar{\sigma}_y$ and $\Delta\bar{\tau}_{xy} = 0$.

Inside the boundary layer, it is expedient to express the thermal stresses in terms of x_n and x_t, where Ox_nx_t is the local coordinate frame with the origin at an arbitrary point, O, of the contour of a film, and x_n and x_t are, respectively, normal and tangential directions at O, with respect to the contour. In this case, Eqs. (2.25)-(2.79) can be reduced to the following equations:

$$\frac{d^2\left(\Delta\bar{\sigma}_{x_n}\right)}{dx_n^2} = \frac{k^2}{l_x^2} \Delta\bar{\sigma}_{x_n} + F\Delta T \quad , \tag{4.4}$$

$$\Delta\bar{\sigma}_{x_t} = v_f \Delta\bar{\sigma}_{x_n} - (\alpha_f - \alpha_s) E_f \Delta T$$
$$\left(\Delta\bar{\tau}_{x_n x_t} = 0 \quad , \qquad \Delta v_0 = \alpha_s x_t \Delta T \quad , \qquad \Delta u_0 = \alpha_s x_n \Delta T\right) \quad , \tag{4.5}$$

$$\tau_{x_n} = t\frac{d\bar{\sigma}_{x_n}}{dx_n} \tag{4.6}$$

The solution to these equations satisfying the boundary condition, $\Delta\bar{\sigma}_{x_n} = 0$ when $x = 0$ (on the film contour) and approaching toward the stress field given by Eqs. (4.1)-(4.3), when $x_n \to \infty$, is easy to find in the following form:

$$\bar{\sigma}_{x_n} = \int_{T_0}^{T} \frac{F(T)}{[k(T)/l_x]^2}\left(e^{-x_n[k(T)/l_x]} - 1\right) dT \quad , \tag{4.7}$$

$$\tau_{x_n} = -t\int_{T_0}^{T} \frac{F(T)}{[k(T)/l_x]} \exp\left(-\frac{x_n k(T)}{l_x}\right) dT \quad . \tag{4.8}$$

The width of the boundary layer is roughly equal to

$$\frac{2l_x}{k(T)} = 2\sqrt{\frac{tt_b E_f}{G_s(1-v_f^2)}} \tag{4.9}$$

While x_n is increasing, τ_{xn} monotonously decreases toward zero when $x_n \to \infty$, and $\bar{\sigma}_{x_n}$ monotonously increases toward the constant maximum defined by Eqs. (4.1) and (4.2). Maximum values of τ_{x_n} and $\bar{\sigma}_{x_n}$ follow:

$$\left(\bar{\sigma}_{x_n}\right)_{max} = -t\int_{T_0}^{T} \frac{F(T)dT}{k(T)/l_x^2} \quad (x_n \to \infty) \quad , \tag{4.10}$$

$$\left(\tau_{x_n}\right)_{max} = -\int_{T_0}^{T} \frac{F(T)dT}{[k(T)/l_x]^2} \quad (x_n = 0) \quad . \tag{4.11}$$

Here, F(T) and k(T) are defined by Eqs. (3.4) and (3.3), respectively.

5. PLASTIC YIELDING OF A THIN FILM: HILLOCK FORMATION

A metal film is elastic until it yields. Yielding begins at a certain temperature difference, T - T_0, when the second invariant of the stress deviator achieves a critical value:[6]

$$\overline{\sigma}_x^2 + \overline{\sigma}_y^2 - \overline{\sigma}_x \overline{\sigma}_y + 3\overline{\tau}_{xy}^2 + 3\tau_y^2 = \sigma_s^2 \quad . \tag{5.13}$$

Here, σ_s is the yielding stress under simple tension or compression.

According to the solution of Section IV, the yielding can begin either on the contour of a thin film or inside the film.(outside the boundary layer). The second case holds when $\left(\overline{\sigma}_{x_n}\right)_{max}$ in Eq. (4.10) achieves σ_s first.

We consider plastic yielding of a thin film in the most important case of large k at

$$\frac{\partial}{\partial x}\frac{\Delta u_0}{\Delta T} = \frac{\partial}{\partial y}\frac{\Delta v_0}{\Delta T} = \alpha_s \quad , \quad \frac{\partial}{\partial x}\frac{\Delta v_0}{\Delta T} = \frac{\partial}{\partial y}\frac{\Delta u_0}{\Delta T} = 0 \quad , \tag{5.2}$$

in Eqs. (4.1)-(4.3), when the following uniform biaxial stress,

$$\begin{gathered} \overline{\sigma}_x = \overline{\sigma}_y = \int_{T_0}^{T} \frac{E_f(T)}{1-\nu_f(T)}\left[\alpha_s(T) - \alpha_f(T)\right] dtT \\ \left(\overline{\tau}_{xy} = 0 \, , \, \tau_y \tau_x = 0\right) \quad , \end{gathered} \tag{5.3}$$

holds in the thin film (except for the boundary layer) before yielding occurs. It is reasonable to assume that the following equations:

$$\overline{\sigma}_x = \overline{\sigma}_y = \sigma \quad , \quad \overline{\tau}_{xy} = 0 \quad , \quad \tau_x = \tau_y = \tau \quad , \tag{5.4}$$

are valid for the total plastic yielding of the film (for sufficiently large T - T_0). Using the condition of biaxiality, Eq. (5.4), in the yielding criterion, Eq. (5.1), we obtain

$$\sigma^2 + 6\tau^2 = \sigma_s^2 \quad . \tag{5.5}$$

According to Eqs. (2.6) or (2.7) the equation of equilibrium has the following form:

$$t\frac{d\sigma}{dr} = \tau \qquad (5.6)$$

Here, *r* is the radial distance from a certain coordinate origin.

Let us introduce the new function, *g(r)* :

$$\sigma = \sigma_s \cos g(r) \quad , \quad \tau = \frac{1}{\sqrt{6}}\sigma_s \sin g(r) \qquad (5.7)$$

The yielding criterion, Eq. (5.5), is satisfied by Eq. (5.7), and substituting σ and τ in Eq. (5.6) by Eq. (5.7) provides the following equation:

$$\left(t\sqrt{6}\frac{dg}{dr} + 1\right)\sin g(r) = 0 \qquad (5.8)$$

This equation has the following two solutions:

$$\begin{aligned} &\sin g(r) = 0 \quad g(r) = \pi n \quad (n = 0, \pm 1, \pm 2, \cdots) \\ &\sigma = \pm\sigma_s, \quad \tau = 0 \quad , \end{aligned} \qquad (5.9)$$

and

$$g = -\frac{r}{t\sqrt{6}} + C$$

$$\sigma = \sigma_s \cos\left(C - \frac{r}{t\sqrt{6}}\right), \; \tau = \frac{1}{\sqrt{6}}\sigma_s \sin\left(C - \frac{r}{t\sqrt{6}}\right) \qquad (5.10)$$

Here C is an arbitrary constant. Suppose that the boundary, $r = r_H$, of a round domain, $r < r_H$, is free of tractions:

when $\quad r = r_H, \quad \sigma = 0 \qquad (5.11)$

Using Eq. (5.11) in Eqs. (5.10), we obtain

$$C = \frac{\pi}{2} + \frac{r_H}{t\sqrt{6}} \quad ,$$

and the second solution, Eq. (5.10), becomes

$$\sigma = \sigma_s \sin\frac{r_H - r}{t\sqrt{6}} \quad , \quad \tau = \frac{\sigma_s}{\sqrt{6}}\cos\frac{r_H - r}{t\sqrt{6}} \qquad (5.12)$$

In the process of cooling or heating, this solution, Eq. (5.12), has developed from the original elastic solution, Eq. (5.3), where $\overline{\sigma}_x = \overline{\sigma}_y = \sigma = \sigma_s, \tau = 0$ at the initiation of yielding.

It is natural to assume that the condition

$$\sigma = \sigma_s , \qquad \tau = 0 \qquad , \qquad (5.13)$$

is valid at the center of the round domain, $r = 0$.

Using Eq. (5.12) we find that the condition of continuity, Eq. (5.13), can be satisfied if

$$r_H = \pi t\sqrt{\frac{3}{2}}\, t = 3.8476496t \qquad (5.14)$$

This is the minimal r_H meeting the condition, Eq. (5.13); other r_H's satisfying the same condition are

$$r_H = \pi t\sqrt{3/2} + 2\pi n t\sqrt{6} \quad (n = 1,2,3,\cdots) \qquad (5.15)$$

For large n, the solution provided by Eqs. (5.12) and (5.15) approaches asymptotically to the uniform solution, Eq. (5.9), in the middle region that extends without limits, when n is increasing.

The infinite series of the solutions constructed represent all possible stationary states of plastic yielding equilibrium of a thin metal film. They probably provide the most substantiated description of successive morphological changes occurring in thin metal films in the process of cooling or heating.

At first, the uniform solution, Eq. (5.9), is valid. However, the uniform yielding is unstable in the post-critical stage[7].

The instability transforms the film condition to the solution. Eqs. (5.12) and (5.15), with n corresponding to the r_H nearest to the original in-plane size of the film.

As a matter of fact, the hillocks must initially have the form of hexagons, which can congruently cover the plane of a thin film and maximize the released free energy[8,9]. A circular form of hillocks is understood as a certain approximation to reality.

6. CONCLUSION TO PART 1

The theory constructed opens a door for predictive physical analysis of thermal stresses in thin films. The abundance of parameters significantly reduces the role of numerical experiments done in this area earlier without the analytical theory.

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PART 2
THE THEORY OF THERMAL STRESSES IN THIN BONDING LAYERS

Thin bonding layers made of solders or metal-filled adhesives are widely used in electronics. They are mostly responsible for the integrity and reliability of computers and other electronic devices. Major concerns are due to thermal stresses arising in the process of electronic packaging. In Part 2, the analytical theory of thermal stresses is constructed under some natural simplifying assumptions. The assumptions include the thermoelastic behavior of the bonded materials and the thermoelastic-plastic behavior of a bonding layer after the latter is deposited and the composite system is cooled to an operational temperature. The closed system of governing partial differential equations for thermal stresses in a thin bonding layer is derived for any in-plane shape of the layer. Some particular problems are solved in an explicit form and the implication of the solutions for the prediction of planar voids and cracks formation is discussed.

1. INTRODUCTION

Suppose, for example[1], that an Au-Sn solder connecting an alumina ceramic substrate and a Si or Ga-As die (chip), is deposited at 280°C in the form of a thin layer, and then the composite material is cooled to room temperature of operation. The coefficients of the thermal expansion of the Au-Sn eutectic alloy, alumina and silicon are 15.9, 6.7 and $2.8 \times 10^{-6}/°C$ respectively. While the Au-Sn tries to shrink, the alumina substrate and silicon die restrict it from doing so; hence, in cooling, the Au-Sn is under tension. These thermal stresses may induce plastic yielding and microcracking of the bonding layer producing a great void or planar crack that can split the chip or otherwise disintegrate the system[2-6].

In Part 2 the analytical theory of thermal stresses in a thin bonding layer is constructed subject to the following assumptions:

(1) The thickness of a layer is much smaller than the thickness of a die and any in-plane dimension of the layer and bonded materials.

(2) No shear or open-mode cracks are formed during the deformation process by cooling/heating (ideal bonding).

(3) The materials of the substrate and die are homogeneous, isotropic, and elastic.

(4) The material of the bonding layer is homogenous, isotropic and linearly thermoelastic-ideally plastic.

This treatment is based on the approach advanced earlier as applied to simpler problems[7,8].

The literature on thermal stresses is ample (see, for example, Refs. 9-19 on the subject). The novel features of the present approach compared with the previous results of other author as follows.

(1) The approach utilizing the asymptotic idea of a boundary layer from hydrodynamics is a rigorous and general method of mathematical physics. It leads to the closed system of governing partial differential equations for all three components of the peeling thermal stress in a thin bonding layer in terms of two in-plane coordinates of the layer (Sec. II).

(2) The equation system is derived for any in-plane shape of the layer and is formulated in terms of stress increments as some functions of temperature. This allows one to consider thermal expansions and elastic properties of the constituent materials as some arbitrary functions of temperature.

(3) The solution to the general equation system is shown to generally split into two solutions-one describing the uniform field inside and in-plane domain, and the other describing the trim zone near the boundary of the domain (Saint Venant effect zone or boundary layer). The first solution is similar to a potential inviscid flow, and can also be found by elementary means. The second is similar to the viscous flow in a boundary layer, and can often be found analytically for the material parameters being arbitrary functions of temperature (Secs. III and IV). Analytical results for the Saint Venant effect zone in a thin bonding layer have been unknown to this author.

(4) The well-developed plastic yielding a thin bonding layer in the internal domain is considered using the classic limit analysis of thermal stresses (Sec. V).

Some numerical examples demonstrating the internal zone and boundary layer solutions are given in Sec. VI.

2. SYSTEM OF GOVERNING EQUATIONS

A. Thin bonding layer

Consider a thin bonding layer between a substrate and die (Fig. 1). The plane, $z = 0$, is chosen along the flat bonding layer—substrate interface and free surface of the substrate. The x axis is in a cross section of the bonding layer which can have an arbitrary form in planar view. The x, y, and z make up a Cartesian coordinate frame.

The bonding layer—substrate and bonding layer—die interfaces are ideally bonded so that all displacements and the stresses; σ_z, τ_{zx} and τ_{zy}, are continuous across the interfaces. The following designations are made:

$$\tau_x^- = \tau_{zx} \text{ at } z = 0; \ \tau_y^- = \tau_{zy} \text{ at } z = 0$$
$$\tau_x^+ = \tau_{zx} \text{ at } z = t; \ \tau_y^+ = \tau_{zy} \text{ at } z = t \tag{2.1}$$

Here t is the bonding layer thickness.

In what follows, the variation of the stress, σ_z, is considered negligibly small in both a thin bonding layer and boundary zones in a die and substrate influenced by the thin bonding layer and located near the latter. Therefore, the equilibrium equation with respect to the z axis is not essential and can be omitted.

Consider the equilibrium equations with respect to the x and y axes, and let one integrate them over z from $z = 0$ to $z = t$. Using Eq. (2.1) we derive

$$\frac{\partial \bar{\sigma}_x}{\partial x} + \frac{\partial \bar{\tau}_{xy}}{\partial y} = -\frac{\tau_x^+ - \tau_x^-}{t}, \tag{2.2}$$

$$\frac{\partial \bar{\sigma}_y}{\partial y} + \frac{\partial \bar{\tau}_{xy}}{\partial x} = -\frac{\tau_y^+ - \tau_y^-}{t}, \tag{2.3}$$

Here, $\bar{\sigma}_x(x,y), \bar{\sigma}_y(x,y)$, and $\bar{\tau}_{xy}(x,y)$ are corresponding mean stresses in a thin bonding layer:

$$\bar{\sigma}_x = \frac{1}{t}\int_0^t \sigma_x dz, \quad \bar{\sigma}_y = \frac{1}{t}\int_0^t \sigma_y dz, \quad \bar{\tau}_{xy} = \frac{1}{t}\int_0^t \tau_{xy} dz \tag{2.4}$$

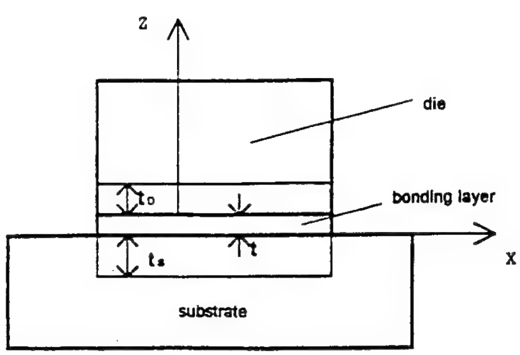

FIG. 1. Schematic representation of a substrate—bonding layer—die composite cross section.

Prior to when yielding occurs, the bonding layer material is thermoelastic and satisfies the following incremental Hooke's law equations:

$$\frac{\partial(\Delta U)}{\partial x} = \frac{\Delta \bar{\sigma}_x - \nu\Delta\left(\bar{\sigma}_y + \sigma_z\right)}{E} + \alpha\Delta T \ , \tag{2.5}$$

$$\frac{\partial(\Delta V)}{\partial y} = \frac{\Delta \bar{\sigma}_y - \nu\Delta\left(\bar{\sigma}_x + \sigma_z\right)}{E} + \alpha\Delta T \ , \tag{2.6}$$

$$\frac{\partial(\Delta U)}{\partial y} + \frac{\partial(\Delta V)}{\partial x} = \frac{\Delta \bar{\tau}_{xy}}{G} \tag{2.7}$$

Here, $U\ (x,\ y)$ and $V\ (x,\ y)$ are mean displacement components along the x and y axes, respectively (in a thin bonding layer), E is Young's modulus, G is the shear modulus, ν is Poisson's ratio, and α is the thermal expansion coefficient. The subscript s will correspond to the substrate material, subscript D to that of the die, and no subscript will correspond to the solder. The value of T denotes the temperature with respect to a certain reference temperature when all thermal stresses equal zero. (In the example of Section 1, the reference temperature is the temperature of the electronic packaging when the solder is deposited on Si, and the chip is attached). Detecting a reference state is often a crucial point in the theory of generation of residual stresses[20]. The symbol Δ designates the infinitesimal increment of a quantity corresponding to the increment $\Delta\ T$ of the temperature. The parameters α, E, G, and ν, are, generally, some functions of the temperature. Equations (2.2) and (2.3) also hold for stress increments.

B. Substrate and die

A thin bonding layer influences the stress and strain field of a substrate and the die in certain boundary zones in the neighborhood of the bonding layer. Outside the boundary zones, the stress and strain field are not perturbed by a thin bonding layer; hence, they are the same field as with zero thickness bounding layer. We assume that the boundary zone occupies the domain, $0 > z > -t_s$,, $0 < x < l_x$, and $0 < y < l_y$, in the substrate, and $t_D > z > 0$, $0 < x < l_x$ and $0 < y < l_y$, in the die, in Fig. 1, where t_s and t_D are the thickness of the boundary zone in the substrate and die, respectively, and l_x and l_y are some planar dimensions of the rectangular bonding layer. The values of t_s and t_D, if unknown from the physical formulation of a problem, are considered as fitting parameters, which can be chosen to better approximate the function of primary interest. For example, in the case of a rigid, strip shaped bonding layer, it was determined[7] that from a comparison with the exact solution, t_s and t_D are roughly equal one-sixth of the strip width.

Due to the small thickness of the bonding layer, we can ignore the bending stresses in the layer, so that the thin bonding layer can induce in the substrate and die the shear stresses, τ_{xz} and τ_{yz}, and in-plane displacements, u and v, and in-plane stresses, σ_x, σ_y and τ_{xy}.

Using the method of Section IIB of reference[8] we derive

$$\Delta U = (\Delta u_0)_S + \frac{t_S \Delta \tau_x^-}{G_S} = (\Delta u_0)_D - \frac{t_D \Delta \tau_x^+}{G_D} \tag{2.8}$$

$$\Delta V = (\Delta v_0)_S + \frac{t_S \Delta \tau_y^-}{G_S} = (\Delta v_0)_D - \frac{t_D \Delta \tau_y^+}{G_D} \tag{2.9}$$

Here, $(\Delta u_o)_s$, $(\Delta v_o)_s$, $(\Delta u_o)_D$, and $(\Delta v_o)_D$ are the increments of corresponding displacements, u and v, in the substrate and die of the field unperturbed by the thin bonding layer. These functions of x and y should be determined from the analysis of the thermal stress and stress field in the bonded substrate—die system with a bonding layer of zero thickness. In the following, they are considered given. The stress, σ_z (x, y), in Eqs. (2.5) and (2.6) should also be determined from the analysis of the same system with a bonding layer of zero thickness.

From the bonding condition on the substrate—die interface with a zero-thickness bonding layer, it follows that

$$(\Delta u_o)_s = (\Delta u_o)_D = \Delta u_o, \;\; (\Delta v_o)_s = (\Delta v_o)_D = \Delta v_o, \tag{2.10}$$

and hence from Eqs. (2.8) and (2.9) we derive

$$t_s \; G_D \; \Delta \tau_x^- = - \; t_D \; G_s \; \Delta \tau_x^+ \tag{2.11}$$

$$t_s \; G_D \; \Delta \tau_y^- = - \; t_D \; G_s \; \Delta \tau_y^+ \tag{2.12}$$

Writing Eqs. (2.2) and (2.3) in the incremental form and substitute $\Delta\tau_x^+$ and $\Delta\tau_y^+$ for Eqs. (2.11) and (2.12) is obtained:

$$\frac{1}{t}\Delta \tau_x^- = \frac{t_D G_s}{t_D G_s + t_s G_D} \left[\frac{\partial}{\partial x}\left(\Delta \bar{\sigma}_x\right) + \frac{\partial}{\partial y}\left(\Delta \bar{\tau}_{xy}\right) \right] \tag{2.13}$$

$$\frac{1}{t}\Delta \tau_y^- = \frac{t_D G_s}{t_D G_s + t_s G_D} \left[\frac{\partial}{\partial y}\left(\Delta \bar{\sigma}_y\right) + \frac{\partial}{\partial x}\left(\Delta \bar{\tau}_{xy}\right) \right] \tag{2.14}$$

Substituting ΔU and ΔV in Eqs. (2.5), (2.6) and (2.7) for Eqs. (2.8) and (2.9), one derives

$$\frac{\Delta\bar{\sigma}_x - \nu\Delta\bar{\sigma}_y}{E} = \frac{\nu\Delta\sigma_z}{E} + \frac{t_s}{G_s}\frac{\partial(\Delta\tau_x^-)}{\partial x} + \frac{\partial(\Delta u_o)}{\partial x} - \alpha\Delta T \tag{2.15}$$

$$\frac{\Delta\bar{\sigma}_y - \nu\Delta\bar{\sigma}_x}{E} = \frac{\nu\Delta\sigma_z}{E} + \frac{t_s}{G_s}\frac{\partial(\Delta\tau_y^-)}{\partial y} + \frac{\partial(\Delta v_o)}{\partial y} - \alpha\Delta T \tag{2.16}$$

$$\frac{\Delta\bar{\tau}_{xy}}{G} = \frac{t_s}{G_s}\left[\frac{\partial(\Delta\tau_x^-)}{\partial y} + \frac{\partial(\Delta\tau_y^-)}{\partial x}\right] + \frac{\partial(\Delta u_o)}{\partial y} + \frac{\partial(\Delta v_o)}{\partial x} \tag{2.17}$$

Substituting $\Delta\tau_x^-$ and $\Delta\tau_y^-$ in Eqs. (2.15) through (2.17) by Eqs. (2.13 and (2.14) provides

$$\partial^2\frac{(\Delta\bar{\sigma}_x)}{\partial x^2} + \frac{\partial^2(\Delta\bar{\tau}_{xy})}{\partial x\partial y} = \frac{t_D G_s + t_s G_D}{tt_s t_D}\left[\frac{\Delta\bar{\sigma}_x - \nu\Delta\bar{\sigma}_y}{E} - \frac{\nu\Delta\sigma_z}{E} - \frac{\partial(\Delta u_o)}{\partial x} + \alpha\Delta T\right], \tag{2.18}$$

$$\frac{\partial^2(\Delta\bar{\sigma}_y)}{\partial y^2} + \frac{\partial^2(\Delta\bar{\tau}_{xy})}{\partial x\partial y} = \frac{t_D G_s + t_s G_D}{tt_s t_D}\left[\frac{\Delta\bar{\sigma}_y - \nu\Delta\bar{\sigma}_x}{E} - \frac{\nu\Delta\sigma_z}{E} - \frac{\partial(\Delta v_o)}{\partial y} + \alpha\Delta T\right], \tag{2.19}$$

$$\frac{\partial^2}{\partial x\partial y}\left(\Delta\bar{\sigma}_x + \Delta\bar{\sigma}_y\right) + \frac{\partial^2(\Delta\bar{\tau}_{xy})}{\partial x^2} + \frac{\partial^2(\Delta\bar{\tau}_{xy})}{\partial y^2} = \frac{t_D G_s + t_s G_D}{t\, t_s t_D}\left[\frac{\Delta\bar{\tau}_{xy}}{G} - \frac{\partial(\Delta u_o)}{\partial y} - \frac{\partial(\Delta v_o)}{\partial x}\right]. \tag{2.20}$$

The system of three partial differential equations, Eqs. (2.18)—(2.20), will serve to help one find the increments of thermal elastic stresses $\bar{\sigma}_x$, $\bar{\sigma}_y$, and $\bar{\tau}_{xy}$ in a bonding layer in terms of x and y. On the boundary of a bonding domain, the corresponding normal and shear stresses (tractions) vanish; for example, for a rectangular domain we have

$$\begin{aligned} &x = 0, x = l_x \quad \Delta\bar{\sigma}_x = \Delta\bar{\tau}_{xy} = 0 \\ &y = 0, y = l_y \quad \Delta\bar{\sigma}_y = \Delta\bar{\tau}_{xy} = 0 \end{aligned} \tag{2.21}$$

In the limiting case when G_b tends towards zero, the equation system, Eqs. (2.18) through (2.20), coincides with that for a thin film[8]. In the latter case, the σ_z is a known normal load on the thin film surface, which is assumed to be zero in ref. 8. The σ_z (x, y), u_o $(x, y$, and v_o (x, y) in Eqs. (2.18) through (2.20) are the values of corresponding stress and displacements on the die-substrate interface when the thickness of the bonding layer equals zero.

If one considers the equilibrium equation with respect to the z axis and integrates it over z from $z = 0$ to $z = t$, the application of the Hooke's law equation for τ_{xz} and τ_{yz} yields

$$[\sigma_z] = -G\left(\left[\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right] + t\bar{\kappa}\right) \tag{2.22}$$

$$\bar{\kappa} = \frac{1}{t}\int_0^t \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2}\right) dz \tag{2.23}$$

Here, u, v, and w are the Cartesian coordinates of the displacement vector, $\bar{\kappa}$ is the mean curvature of the bonding layer, and $[A\ (x,y,z)]$ is the discontinuity of A across the bonding layer, that is, $[A] = A\ (x,y,t) - A\ (x,y,o)$. From Eqs. (2.22) and (2.23), it follows that $[\sigma_z]$ tends towards zero when $t \rightarrow 0$, because u and v are continuous along the bonded die—substrate interface.

For small t, the variation of σ_z across the bonding layer is of the order of the negligible variation of σ_x and σ_y. . Hence, the bending effects of the thin bonding layer can be neglected; however, the bending of die and substrate, if it is essential, is taken into account by the functions, u_o (x,y), v_o (x,y) and σ_z (x,y), in Eqs. (2.18) through (2.20).

3. A STRIP-SHAPED THIN BONDING LAYER

Consider the case when a bonding layer is deposited in the form of an infinite strip, $|x| < l_x$, of width $2l_x$ (when $l_y >> l_x$). In this case, due to the symmetry, the $\Delta\bar{\sigma}_x$ and $\Delta\bar{\sigma}_y$ are some functions of only x, and $\bar{\tau}_{xy} = 0$, so that the governing equation system, Eqs. (2.18) through (2.20), become

$$\frac{d^2(\Delta\bar{\sigma}_x)}{d_x^2} = \frac{k^2}{\text{liter}_x^2}\Delta\bar{\sigma}_x + F\Delta T \ . \tag{3.1}$$

Here,

$$k^2 = \frac{\text{liter}_x^2(1-\nu^2)(t_D G_S + t_S G_D)}{t\, t_S t_D E} \ , \tag{3.2}$$

$$F = \frac{k^2 E}{\text{liter}_x^2(1\_\nu^2)}\left[\alpha(1+\nu) - \frac{\nu(1+\nu)}{E}\frac{\Delta\sigma_z}{\Delta T} - \frac{\partial}{\partial x}\frac{\Delta u_0}{\Delta T} - \nu\frac{\partial}{\partial y}\frac{\Delta v_0}{\Delta T}\right] \tag{3.3}$$

$$\Delta\bar{\sigma}_y = \nu(\Delta\bar{\sigma}_x + \Delta\sigma_z) + E\frac{\partial}{\partial y}(\Delta v_0)\_\alpha E\Delta T \ , \tag{3.4}$$

$$\frac{\partial(\Delta u_0)}{\partial y} + \frac{\partial(\Delta v_0)}{\partial x} = 0 \tag{3.5}$$

To find u_o, v_o, and σ_z, let us confine ourselves to a simple case of a die of rectangular parallelepiped shape attached to a substrate of an analogous shape along one face (Fig. 2). The dimensions of the die and substrate along the x axis are assumed to be small as compared to their dimensions along the y and z axes. An elementary analysis of thermal stresses and strains in this composite system (with a zero thickness bonding layer) provides the following results:

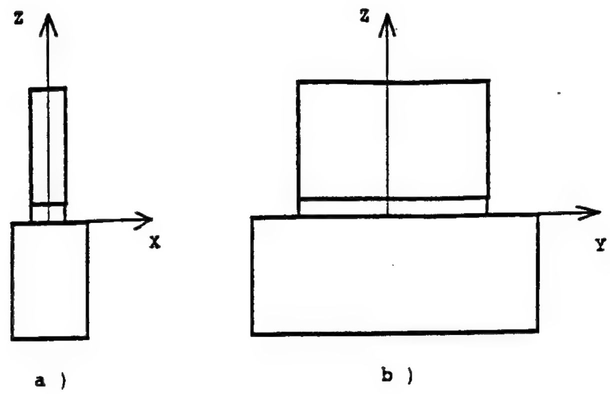

FIG. 2. A die-substrate systems: (a) a cross section, and (b) a lateral view.

$$\Delta u_0 = x\Delta T\left[\alpha_D - \nu_D(1+\nu_S)\frac{\alpha_S - \alpha_D}{\nu_S - \nu_D}\right], \tag{3.6}$$

$$\Delta v_0 = y\Delta T\left[\alpha_D + (1+\nu_S)\frac{\alpha_S - \alpha_D}{\nu_S - \nu_D}\right], \tag{3.7}$$

$$\Delta \sigma_z = 0 \tag{3.8}$$

while the thermal stresses in the die and substrate are as follows:

$$\Delta \sigma_y^D = (1+\nu_S)\frac{\alpha_S - \alpha_D}{\nu_S - \nu_D} E_D \Delta T \tag{3.9}$$

$$\Delta \sigma_y^s = (1+\nu_D)\frac{\alpha_S - \alpha_D}{\nu_S - \nu_D} E_S \Delta T \tag{3.10}$$

The remaining components of the thermal stress tensor equal zero.

The bending in the *Oyz* plane can be neglected because the dimension of the die and substrate along the z axis is of the same or larger order then the dimension along the y axis (Fig. 2). In this particular case, F in Eq. (3.1) is the following constant:

$$F = \frac{k^2 E}{\text{liter}_x^2(1-\nu)}\left[\alpha - \alpha_D + (\nu_D - \nu)\frac{1+\nu_S}{1+\nu}\,\frac{\alpha_S - \alpha_D}{\nu_S - \nu_D}\right] \tag{3.11}$$

The solution to Eq. (3.1) meeting the boundary condition, $\Delta\bar{\sigma}_x = 0$, when $x = \pm l_x$, after integrating it over T, becomes

$$\bar{\sigma}_x = \mathrm{liter}_x^2 \int_{T_o}^{T} \frac{F(T)}{k^2(T)} \left(\frac{\cosh(xk(T)xk(T)/\mathrm{liter}_x)}{\cosh k(T)} - 1 \right) dT \tag{3.12}$$

Here, T_o is the reference temperature of electronic packaging when $\bar{\sigma}_x = 0$. The $F(T)$ and $k(T)$ are defined by Eqs. (3.2) and (3.11) where E, ν, ν_s, ν_D, α, α_s, α_D, G_s, and G_D are some known functions of T. The $\bar{\sigma}_y$ is defined by Eqs. (3.4, (3.7), (3.8), and (3.12) as follows

$$\bar{\sigma}_y = \int_{T_o}^{T} \nu(T) \frac{\Delta\bar{\sigma}_x}{\Delta T} dT + \int_{T_o}^{T} E \left[\alpha_D - \alpha + (1 + \nu_S) \frac{\alpha_S - \alpha_D}{\nu_S - \nu_D} \right] dT \tag{3.13}$$

The thermal stresses appear to substantially depend, not only on the differences in the thermal expansion coefficient of die, substrate and bonding layer materials, but also on the difference of Poisson's ratio of the die and substrate materials.

4. SOLUTION FOR LARGE k

The case of large k defined by Eq. (3.2) is of importance for very thin bonding layers, which is realized, for example, when $l_x^2 >> t\, t_s$, and $l_x^2 >> t\, t_D$, and G_s and G_D are of the order of E. In this case, the solution to the governing equation system, Eqs. (2.18) through (2.20), constitutes a narrow boundary layer that borders the contour of a bonding area. Everywhere inside the arbitrary contour of the area, except for the boundary layer, the solution is given by the following equations:

$$\Delta\bar{\sigma}_x - \nu\Delta\bar{\sigma}_y = E\left(-\alpha\Delta T + \frac{\nu}{E}\Delta\sigma_z + \frac{\partial}{\partial x}(\Delta u_o)\right) \tag{4.1}$$

$$\Delta\bar{\sigma}_y - \nu\Delta\bar{\sigma}_x = E\left(-\alpha\Delta T + \frac{\nu}{E}\Delta\sigma_z + \frac{\partial}{\partial y}(\Delta u_o)\right) \tag{4.2}$$

$$\Delta\bar{\tau}_{xy} = G\left(\frac{\partial(\Delta u_o)}{\partial y} + \frac{\partial(\Delta v_o)}{\partial x}\right) \tag{4.3}$$

In a particular case of Section III, described by Fig. 2 and Eqs. (3.6) through (3.10), we have

$$\frac{1}{E}\frac{\Delta\bar{\sigma}_x}{\Delta T} = \frac{\alpha_D - \alpha}{1 - \nu} + \frac{(\nu - \nu_D)(1+\nu_s)}{1-\nu^2}\frac{\alpha_s - \alpha_D}{\nu_s - \nu_D}\ , \tag{4.4}$$

$$\frac{1}{E}\frac{\Delta\bar{\sigma}_y}{\Delta T} = \frac{\alpha_D - \alpha}{1 - \nu} + \frac{(1 - \nu\nu_D)(1+\nu_s)}{1-\nu^2}\frac{\alpha_s - \alpha_D}{\nu_s - \nu_D}\ , \tag{4.5}$$

$$\Delta\bar{\tau}_{xy} = 0 \tag{4.6}$$

Inside the boundary layer, it is expedient to express the thermal stresses in terms of x_n and x_t, where $0x_n\ x_t$ is the local coordinate frame with the origin at an arbitrary point, 0, of the contour of a bonding area, and x_n and x_t are, respectively, normal and tangential directions at 0, with respect to the contour. In this case, Eqs. (2.18)-(2.20) can be reduced to the following equations:

$$\frac{d^2(\Delta\bar{\sigma}_n)}{dx_n^2} = \frac{k^2}{\text{liter}_n^2}\Delta\bar{\sigma}_n + F_o\,\Delta T\ , \tag{4.7}$$

$$\Delta\bar{\sigma}_t = \nu(\Delta\bar{\sigma}_n + \Delta\sigma_z) + E\frac{\partial(\Delta u_t)}{\partial x_t} - \alpha E\Delta T\ , \tag{4.8}$$

$$k^2 = \frac{\text{liter}_n^2\,(1-\nu^2)(t_D\ G_S + t_s\ G_D)}{t\ t_s\ t_D\ E}\ , \tag{4.9}$$

$$F_o = \frac{k^2 E}{\text{liter}_n^2 (1-\nu^2)} \left[\alpha(1+\nu) - \frac{\nu(1+\nu)}{E} \frac{\Delta\sigma_z}{\Delta T} - \frac{\partial}{\partial x_t} \frac{\Delta u_n}{\Delta T} - \nu \frac{\partial}{\partial x_n} \frac{\Delta u_t}{\Delta T} \right] \tag{4.10}$$

$$\frac{\partial(\Delta u_n)}{\partial x_t} + \frac{\partial(\Delta u_t)}{\partial x_n} = 0 \ , \ \Delta \tau_n^+ = -\frac{t\, t_s G_D}{t_s G_D + t_D G_s} \frac{d(\Delta \bar{\sigma}_n)}{d x_n} \tag{4.11}$$

$$\Delta \bar{\tau}_{tn} = 0 \ , \ \Delta \tau_n^- = \frac{t\, t_D G_s}{t_s G_D + t_D G_s} \frac{d(\Delta \bar{\sigma}_n)}{d x_n} \ , \ \tau_t^+ = \tau_t^- = 0 \tag{4.12}$$

Here, subscripts t and n correspond to the tangential and normal direction respectively. The F_o, l_n and k can be considered to be independent of x_n and x_t. The solution to these equations should satisfy the boundary condition, $\Delta\bar{\sigma}_n = 0$ when $x_n = 0$ (on the contour of a bonding area). When $x_n \rightarrow \infty$, the solution should approach the stress field given by Eqs. (4.1) through (4.3) at the point 0. Solving Eq. (4.7) yields

$$\bar{\sigma}_n = \int_{T_o}^{T} \frac{F_o(T)\, l_n^2(T)}{k^2(T)} \left[e^{-x_n(k(T)/l_n)} - 1 \right] dT \tag{4.13}$$

The F_o (T) is the value of F at the point 0. The width of the boundary layer is roughly equal to

$$\frac{2\, l_n(T)}{k(T)} = 2\sqrt{\frac{t\, t_s t_D E}{(1-\nu^2)(t_D G_s + t_s G_D)}} \tag{4.14}$$

When x_n is increasing, τ_n^+ and τ_n^- monotonously decrease toward zero, and $\bar{\sigma}_n$ increases toward the maximum value

$$(\bar{\sigma}_n)_{max} = \int_{T_o}^{T} \frac{F_o(t)\, \text{liter}_n^2(T)}{k^2(T)} dT \tag{4.15}$$

Maximum values of interface shear stresses, τ_n^+ and τ_n^-, follow:

$$\left(\tau_n^+\right)_{max} = t \int_{T_o}^{T} \frac{t_S \, liter_n F_o G_D}{k(t_S G_D + t_D G_S)} dT \quad (x_n = 0) \tag{4.16}$$

$$\left(\tau_n^-\right)_{max} = -t \int_{T_o}^{T} \frac{t_D \, liter_n F_o G_S}{k(t_S G_D + t_D G_S)} dT \quad (x_n = 0) \tag{4.17}$$

Here, l_n/k and F_o are defined by Eqs. (4.9) and (4.10).

5. PLASTIC YIELDING OF A BONDING LAYER: FORMATION OF PLANAR VOIDS AND CRACKS

A solder bonding layer is elastic until it yields. Yielding begins at a certain temperature difference, $T - T_o$, when the second invariant of the stress deviator achieves a critical value[21]

$$\bar{\sigma}_x^2 + \bar{\sigma}_y^2 + \sigma_z^2 - \bar{\sigma}_x \bar{\sigma}_y - \bar{\sigma}_x \sigma_z - \bar{\sigma}_y \sigma_z + 3 \bar{\tau}_{xy}^2 + 6 \tau^2 = \sigma_S^2 \tag{5.1}$$

where

$$2\tau^2 = \max\left[\left(\tau_{zx}^+\right)^2 + \left(\tau_{zy}^+\right)^2 , \ \left(\tau_{zx}^-\right)^2 + \left(\tau_{zy}^-\right)^2\right] \tag{5.2}$$

Here, σ_s is the yielding stress under simple tension or compression. Yielding can begin either on upper or lower interface of a bonding layer, and either on the contour of a bonding area or inside the latter (outside the boundary layer). The second case holds when $(\bar{\sigma}_n)_{max}$ in Eq. (4.15) achieves σ_s first.

We consider plastic yielding of a bonding layer in the important particular case studied in Section III (Fig. 2):

$$\bar{\tau}_{xy} = 0, \quad \sigma_z = 0, \quad \tau_{yz} = 0 \tag{5.3}$$

Designate that $\bar{\sigma}_x = \sigma$.

For a well-developed plastic yielding, a solder alloy material can be considered incompressible; we thus have[10]

$$\bar{\sigma}_y = \frac{1}{2}\left(\bar{\sigma}_x + \sigma_z\right) \tag{5.4}$$

Additionally, let us assume that

$$\tau_{zx}^{-} = -\tau_{zx}^{+} = \tau \tag{5.5}$$

This condition is particularly satisfied if the thermal and elastic properties of die and substrate materials coincide, and the middle plane of a bonding layer, $z = t/2$, is a plane of symmetry of the problem.

In this case, with the account of Eqs. (5.2) through (5.5) the yielding criterion, Eq. (5.1), becomes

$$3\sigma^2 + 24\tau^2 = 4\sigma_s^2 \ , \tag{5.6}$$

and the equation of equilibrium has the following form:

$$t\frac{d\sigma}{dx} = 2\tau \qquad \left(-\text{liter}_x < x < +\text{liter}_x\right) \tag{5.7}$$

The ends of a bonding layer are free of tractions when:

$$x = \pm l_x \ , \ \sigma = 0 \tag{5.8}$$

The solution to the boundary value problem, Eqs. (5.6) through (5.8) is as follows:

$$\sigma = \frac{2\sigma_s}{\sqrt{3}}\sin\frac{x + \text{liter}_x}{t\sqrt{2}} \ , \tau = \frac{\sigma_s}{\sqrt{6}}\cos\frac{x + \text{liter}_x}{t\sqrt{2}} \ . \tag{5.9}$$

Here, $2l_x$ should be equal to

$$2\,\text{liter}_x = \sqrt{2}\left(\frac{\pi}{2} + \pi n\right)t \ , \tag{5.10}$$

where $n = 0, 1, 2, 3, \ldots$ Particularly, when $n = 0$ we have $2l_x \pi t \sqrt{2}$.

If $2l_x < \pi t \sqrt{2}$, the yielding of the entire bonding area is impossible. In this case, the bonding layer is probably elastic, at least, partially.

If l_x satisfies Eq. (5.10), the stresses, σ and τ, in the bonding layer are periodical functions of x, that is, they form a frozen space wave of length, $2 \pi t \sqrt{2}$, where the tension and compression alternate during a period.

In the middle of every wave of tensile σ the formation of a planar rupture, whose plane is perpendicular to the x axis, is possible. The rupture, if it crosses interface can split a die. It is interesting that the ruptures are periodically located in the bonding layer, on the distance $2 \pi t \sqrt{2}$ from one from another. Between the nearest possible ruptures, right in the middle, σ is zero and τ is maximal. At these points interface slips are possible, which are also periodic with period $\pi t \sqrt{2}$. The ruptures are perpendicular to the x axis and can extend along the y axis through the entire bonding area.

If l_x does not satisfy Eq. (5.10), in a bonding layer, there is probably one segment of length less than $\pi t \sqrt{2}$ which is, at least, partially elastic. The remaining part of the bonding layer is covered by a periodic wave solution, Eq. (5.9).

The interpretation of an analogous periodic solution in Ref. 8 with respect to hillock formation in thin films is probably invalid in what concerns the evolution of hillocks. From the solution, it follows

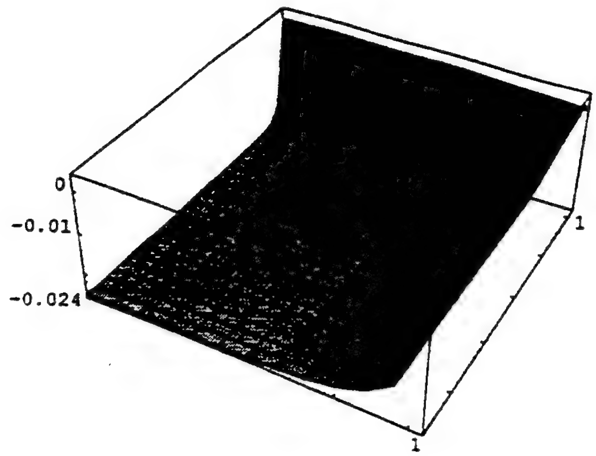

FIG. 3. The sum of principal stresses $\hat{\sigma}_x + \hat{\sigma}_y$ (surface graphics).

that the dimension of the hillocks is one and the same from the beginning of instability during the process of heating and cooling. The latter can only influence on the level of a plastic deformation of a hillock.

6. SOME NUMERICAL EXAMPLES

Equations (2.18) - (2.20) provide the closed system of partial differential equations for increments of thermal stresses, $\Delta\overline{\sigma}_x, \Delta\overline{\sigma}_y$ and $\Delta\overline{\tau}_{xy}$, in a thin bonding layer of an arbitrary in-plane shape. As a numerical example, we consider the rectangular shape of the bonding layer in the cases of $\Delta\sigma_z = 0$, and Δu_0, and Δv_0 given by Eqs. (3.6) and (3.7), see Fig. 2.

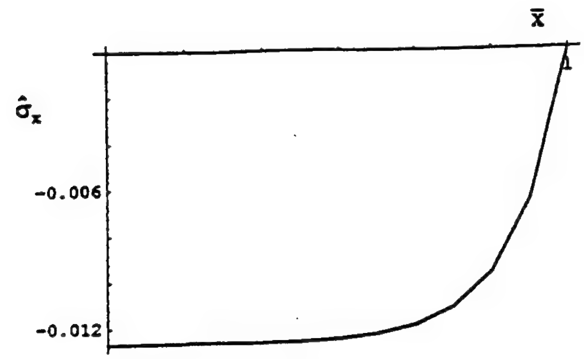

FIG. 4. The $\hat{\sigma}_x$ vs $\bar{x}$ along $\bar{y} = 0$.

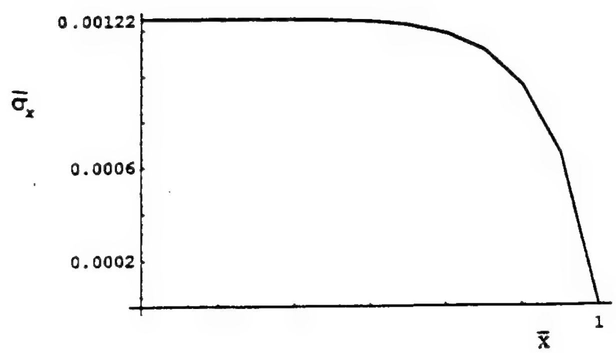

FIG. 5. The $\hat{\sigma}_x$ vs $\bar{x}$ along $\bar{y} = 1$.

Consider the following input data:

gold - - tin (Au-Sn) solder

$\alpha = 15.9 \times 10^{-6}/°C$, $\nu = 0.35$, $G = 30\ GPa$,

$E = 81$ GPa;

alumina (Al_2O_3) substrate

$\alpha_s = 6.7 \times 10^{-6}/°C$, $\nu_s = 0.22$,

$G_s = 160$ GPa, $E_s = 390$ GPa;

silicon (Si) die

$\alpha_D = 2.8 \times 10^{-6}/°C, \quad \nu_D = 0.27,$

$G_D = 150 \text{ GPa}, \quad E_D = 381 \text{ GPa}.$

The bonding layer is assumed to occupy the domain, $|x| < a$ and $|y| < b$, in the xy plane, where

$a = 1.25$ mm, $\quad b = 5$ mm..

The remaining geometrical parameters are chosen to be

$t = 100 \ \mu\text{m}, \quad t_s = t_D = 300 \ \mu\text{m}.$

The change of temperature, from manufacturing to operation, is taken to be

$\Delta T = 200$ °C.

The author did not have detailed data available on the variation of thermal expansion and elastic constants with temperature in this range, therefore, the material parameters were taken as invariable in the present numerical example.

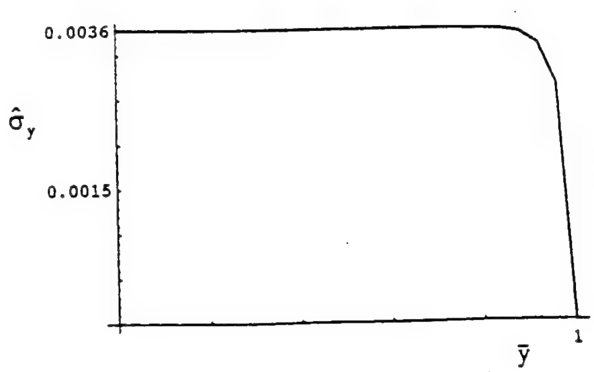

FIG. 6. The $\hat{\sigma}_y$ vs $\bar{y}$ along $\bar{x} = 1$.

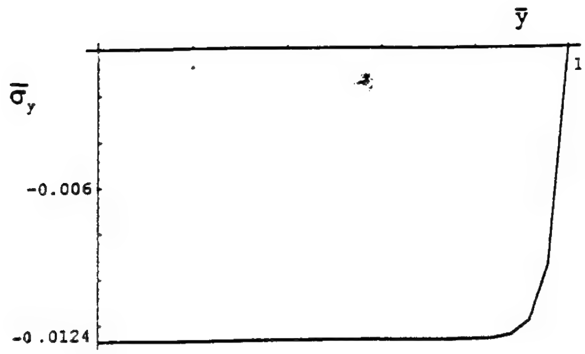

FIG 7. The $\hat{\sigma}_y$ vs $\bar{y}$ along $\bar{x} = 0$.

The calculation was done using *Matematica* and a finite difference model with grid of 25 × 100. The results of the calculation are depicted in Figs. 3-7 for the quarter, $0 < x < a$ and $0 < y < b$, which is sufficient because of symmetry.

The dimensionless values

$$\hat{\sigma}_x = \frac{\Delta\bar{\sigma}_x}{E}, \quad \hat{\sigma}_y = \frac{\Delta\bar{\sigma}_y}{E}, \quad \hat{\tau}_{xy} = \frac{\Delta\bar{\tau}_{xy}}{E}, \quad \bar{x} = \frac{x}{a}, \quad \bar{y} = \frac{y}{b},$$

are used in Figs. 3-7.

Figure 3 shows the three-dimensional graphics of the sum, $\hat{\sigma}_x + \hat{\sigma}_y$, in terms of $\bar{x}$ and $\bar{y}$. It demonstrates the uniform internal solution similar to a potential flow of an inviscid fluid and the boundary layer solution around the boundary of the rectangular domain. Figures 4-7 show the distribution of the characteristic nonzero stresses, $\hat{\sigma}_x$ and $\hat{\sigma}_y$, along the boundary contour and the symmetry lines of the domain.

7. CONCLUSION TO PART 2

Thermal stresses in a bonding layer between a die and substrate can be predicted and analyzed using the equation system constructed. The analytical theory is necessary in this field due to a great number of parameters in the problems of such kind[22].

An analysis of a particular problem discovered that, besides the difference of thermal expansion coefficients, the difference of Poisson's ratio of the die and substrate may also be crucial.

Thermal stresses in a plastic state of a bonding layer are shown to be periodic, which provides a causative background for possible formation of a periodic lattice of planar cracks or voids perpendicular to interfaces.

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PART 3
THE NUMERICAL CODE FOR THERMAL STRESSES IN THIN FILMS AND BONDING LAYERS

Thermal stresses are primarily responsible for morphological changes in thin films, including hillocks, whiskers, and void or pit formations, which present serious problems of reliability in microelectronics. In Part 3, a computerized code for prediction of thermal stresses in thin films is suggested. The closed system of governing partial differential equations for thermal stresses in a thin film is utilized for any in-plane shape of the film. Some numerical experiments are conducted to verify the code.

1. INTRODUCTION

Suppose, for example, [1], that Pb is deposited on a Si substrate at room temperature in the form of a thin film, and then the composite material is cooled to 4.2K where the Pb becomes superconducting. The coefficients of the thermal expansion of Pb and Si are 29.5×10^{-6}°C, respectively. While the Pb tries to shrink the Si substrate restricts it from doing so; hence, in cooling, the Pb is under tension. These thermal stresses may induce plastic yielding of the film and the formation of hillocks [2, 3, 4]. An analogous phenomenon is possible for some semiconducting alloys deposited on a substrate and cooled to the nitrogen temperature where some semiconductors become superconductive. Upon heating the composite back to room temperature, the thin film tends to expand and again is restricted by the substrate. Thus, the thin film is under compression upon heating.

The closed two-dimensional system of governing partial differential equations for thermal stresses in a thin film was earlier derived for any in-plane shape of the film [5] based on ideas

advanced previously for fibers [6]. The work of other investigators in the field on the one-dimensional theory of thermal stresses is acknowledged, too [7-13]. Some general laws of residual stresses and strains are discussed in Ref. [14].

In Part 3, the finite difference analogue model of the governing equation system is formulated for any in-plane shape of the film. Some numerical experiments are conducted for rectangular shapes which enable to reveal two zones, namely, the boundary layer zone on the trim of a film analogous to a viscous layer, and the internal zone similar to a potential flow of a fluid. The materials of a substrate and film are assumed to be homogeneous, isotropic, and linearly thermoelastic.

2. GOVERNING EQUATIONS

Thin film

Consider a thin film deposited on a substrate (Fig. 1). For definiteness, the film is depicted in Fig. 1 in planar view of a rectangular form having dimensions of $2l_x \times 2l_y$. The plane, z = 0, is chosen along the flat film substrate interface and a possible film-unprotected surface of the substrate. The planes, y = 0 and x = 0, coincide with the planes of symmetry. It is assumed that the boundary surface of the thin film at z = t is free of tractions (t is the ;film thickness):

$$\text{when} \quad z = t,\ |x| < l_x,\ |y| < l_y,:\ \sigma_z = \tau_{zx}\ \tau_{zy} = 0\,. \tag{1}$$

The edges of the film are also free of tractions:

$$\text{when} \quad 0 < z < t\ x = \pm l_x\ :\ \sigma_z = \tau_{zx} = 0$$

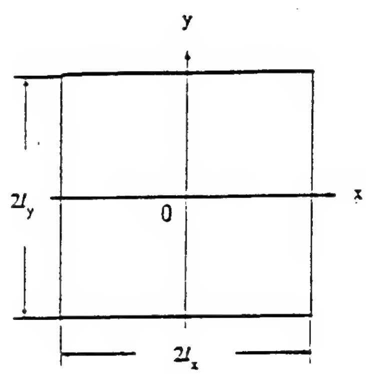
$$\text{when} \quad 0 < z < t\ y = \pm l_y\ :\ \sigma_z = \tau_{yx} = 0. \tag{2}$$

The film-substrate interface at $z = 0$ is ideally bonded so that all displacements and stress σ_z, τ_{zx} and τ_{zy} , are continuous across the interface.

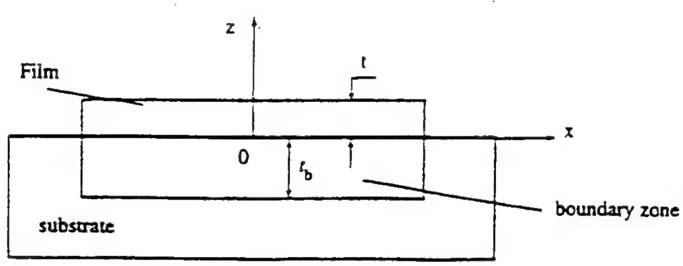
Designate that:

$$\tau_x = \tau_{zx} \quad \text{at} \quad z = 0; \qquad \tau_y = \tau_{zy} \quad \text{at} \quad z = 0. \tag{3}$$

In what follows, stress σ_z is considered negligibly small in both the thin film and substrate boundary zone influenced by the thin film and located near the latter. Therefore, the equilibrium equation with respect to the z axis is not essential and can be omitted. Designate as $\sigma_x(x,y), \sigma_y(x,y)$ and $\bar{\tau}_{x,y}(x,y)$ the corresponding mean stresses in a thin film:



(a)



(b)

Fig. 1. Schematic representation of a film-substrate composite: (a) planar view of a deposited thin film, with dimensions, $2l_x \times 2l_y \times t$; (b) sectional view showing the substrate boundary zone with dimensions, $2l_x \times 2l_{tb}$.

$$\overline{\sigma}_x = \frac{1}{t}\int_0^1 \sigma_x \mathrm{dz}, \overline{\sigma}_y = t\int_0^l \sigma_y \mathrm{dz}, \quad \overline{\tau}_{yx} = \frac{1}{t}\int_0^1 \tau_{xy} \mathrm{dz}, \tag{4}$$

Prior to when yielding occurs, the film material is thermoelastic and satisfies the following incremental Hooke's law equations;

$$\frac{\partial(\Delta U)}{\partial x} = \frac{\Delta\overline{\sigma}_x - \nu_f \Delta\overline{\sigma}_v}{E_f} + \alpha_f \Delta T \tag{5}$$

$$\frac{\partial(\Delta U)}{\partial y} = \frac{\Delta\overline{\sigma}_x - \nu_f \Delta\overline{\sigma}_v}{E_f} + \alpha_f \Delta T \tag{6}$$

$$\frac{\partial(\Delta V)}{\partial y} + \frac{\partial(\Delta V)}{\partial x} = \frac{\Delta \tau_{xv}}{G_f} \tag{7}$$

Here, $U(x, y)$ and $V(x, y)$ are mean displacement components along the x and y axes, respectively (in a thin film), E is Young's modulus, G is the shear modulus, ν is Poisson's ratio and α is the thermal expansion coefficient. Subscript, f, corresponds to the film material. The value of T denotes the temperature with respect to a certain reference temperature when all thermal stresses equal zero. (In the example of the Introduction, the reference temperature is room temperature, at which Pb is deposited on Si.) The symbol, Δ, designates the infinitesimal increment of a quantity in the thermal process of heating or cooling corresponding to the growth, ΔT, of the temperature. The parameters, α, E, G and ν, generally, are some functions of temperature. A thin film influences the stress and strain field of a substrate in a certain zone in the neighborhood of the thin film. Outside the zone, the stress and field is not perturbed by a thin film, hence, it is the same field as without the thin film. This zone occupies the domain $0 > z > -t_b$, $|x| < l_x$ and $|y| < l_y$, in Fig. 1(b) where t_b is the thickness of the zone. The value of t_b, if unknown from

the physical formulation of a problem, is considered as a fitting parameter, which can be chosen to better approximate the function of a primary interest. For example, in the case of a rigid, strip shaped thin film, it was determined that from a comparison with the exact solution, t_b equals one-sixth of the strip width [6]. Because of the small thickness of the thin film, we can ignore the bending stresses in the film. Under these conditions, the thin film can induce in substrate only shear stresses, τ_{xz} and τ_{yz} , and in-plane displacements, u and v, and in-plane stresses, σ_x , σ_y and τ_{xy}.

In the zone of influence in the substrate, it was derived [5].

$$\tau_{xz} = \tau_x (x, y), \quad \tau_{yz} = \tau_y (x, y) \tag{8}$$

$$\Delta u = z\frac{\Delta\tau_x}{G_s} + \Delta U(x,y),$$

$$\Delta v = z\frac{\Delta\tau_y}{G_s} + \Delta V(x,y), \tag{9}$$

Here, subscript, s, corresponds to the substrate material; the Δ is an infinitesimal increment of a quantity in the heating-cooling process corresponding to the growth, ΔT, of the temperature. Moreover, the following compatibility equations should be satisfied:

$$\text{when } z = -t_b: \quad \Delta u = \Delta u_0, \quad \Delta v = \Delta v_0 . \tag{10}$$

$$\text{when } z = -t_b: \quad \Delta u_0 = x\alpha_s\, \Delta T, \quad \Delta v_0 = y\alpha_s\, \Delta T \tag{11}$$

(Here, we also used the symmetry conditions in Fig. 1(a)).

Thus, from Eqs. (9) and (10), it follows that

$$\Delta U = \Delta u_0 + \frac{t_b \Delta\tau_x}{G_s} \tag{12}$$

$$\Delta V = \Delta v_0 + \frac{t_b \Delta \tau_y}{G_s} \tag{13}$$

The governing equation system for $\overline{\sigma}_x, \overline{\sigma}_y$ and $\overline{\tau}_{xy}$ has the following form [5]:

$$\frac{\partial^2(\Delta\overline{\sigma}_x)}{\partial x^2} + \frac{\partial^2(\Delta\overline{\tau}_{xy})}{\partial x\,\partial y} = \frac{G_s}{tt_b}\left[\frac{\Delta\overline{\sigma}_x - \nu_f \Delta\overline{\sigma y}}{E_f} - \frac{\partial(\Delta u_0)}{\partial x} + \alpha_f \Delta T\right] \quad , \tag{14}$$

$$\frac{\partial^2(\Delta\overline{\sigma}_y)}{\partial y^2} + \frac{\partial^2(\Delta\overline{\tau}_{xy})}{\partial x\,\partial y} = \frac{G_s}{tt_b}\left[\frac{\Delta\overline{\sigma}_y - \nu_f \Delta\overline{\sigma y}}{E_f} - \frac{\partial(\Delta v_0)}{\partial y} + \alpha_f \Delta T\right] \quad , \tag{15}$$

$$\frac{\partial^2}{\partial x \partial y}\left(\Delta\overline{\sigma}_x + \Delta\sigma_y\right) + \frac{\partial^2(\Delta\overline{\tau}_{xy})}{\partial x^2} + \frac{\partial^2(\Delta\overline{\tau}_{xy})}{\partial y^2} = \frac{G_s}{tt_b}\left[\frac{\Delta\overline{\tau}_{xy}}{G_f} - \frac{\partial(\Delta u_0)}{\partial y}\right] \quad . \tag{16}$$

The system of three partial differential equations, Eqs. (14) - (16), will serve to find the increments of thermal stresses, $\overline{\sigma}_x, \overline{\sigma}_y$ and $\overline{\tau}_{xy}$, in a thin film in terms of x and y. In view of Eqs. (2) we have:

$$\begin{aligned} x = \pm\, l_x: &\quad \Delta\overline{\sigma}_x = \Delta\overline{\tau}_{xy} = 0 \\ y = \pm\, l_y: &\quad \Delta\overline{\sigma}_y = \Delta\overline{\tau}_{xy} = 0 \end{aligned} \tag{17}$$

Everyone of the three equations (14)-(16) is of the second order. It means that one more boundary condition equation is required to close the formulation of the boundary value problem. It is reasonable to take the following boundary conditions:

$$x = \pm\, l_x: \quad \frac{\partial\sigma_y}{\partial y} + \frac{\partial\tau_{xy}}{\partial y} = 0 \tag{18}$$

$$y = \pm\, l_y: \quad \frac{\partial\sigma_x}{\partial x} + \frac{\partial\tau_{xy}}{\partial y} = 0\,. \tag{19}$$

Physically it means that the shear force on the film border tangential to the film in-plane contour is neglected. The boundary value problem in Eqs. (14)-(19) will be used for the numerical study of thermal stresses in thin films.

3. FINITE DIFFERENCE ANALOGUE OF THE BOUNDARY VALUE PROBLEM

Introduce the following notation:

$$\xi = \frac{x}{t}, \quad \eta = \frac{y}{t} \tag{20}$$

$$f(\xi,\eta) = \frac{\Delta\bar{\sigma}_x}{E_f}, \quad g(\xi,\eta) = \frac{\Delta\bar{\sigma}_y}{E_f}, \quad h(\xi,\eta) = \frac{\Delta\bar{\tau}_{xy}}{E_f} \tag{21}$$

$$\begin{aligned} \lambda &= \frac{tG_s}{t_b E_f}, \quad a = \alpha_f \Delta T - \frac{\partial(\Delta u_0)}{\partial x}, \\ b &= \alpha_f \Delta T - \frac{\partial(\Delta_{v_0})}{\partial y}, \\ c &= \frac{\partial(\Delta u_0)}{\partial y} + \frac{\partial(\Delta v_0)}{\partial x}. \end{aligned} \tag{22}$$

The governing equation system (14) - (16) in this notation can be written as:

$$\frac{\partial^2 f}{\partial \xi^2} + \frac{\partial^2 h}{\partial \xi \partial \eta} = \lambda(f - v_f g + a) \tag{23}$$

$$\frac{\partial^2 g}{\partial \eta^2} + \frac{\partial^2 \eta}{\partial \xi \partial \eta} = \lambda(g - v_f f + b) \tag{24}$$

$$\frac{\partial^2 (f+g)}{\partial \xi \partial \eta} + \frac{\partial^2 h}{\partial \xi^2} + \frac{\partial^2 \mathrm{h}}{\partial \eta^2} = \lambda\left[2(l + v_f)h - c\right] \quad . \tag{25}$$

The boundary condition equations for the rectangular domain $|\xi| < \bar{l}_x \; |\eta| < \bar{l}_y$ of the $\xi\eta$ plane follow from Eqs. (17)-(19):

$$\xi = \pm \bar{l}_x: \quad f = h = 0, \quad \frac{\partial g}{\partial \eta} + \frac{\partial h}{\partial \xi} = 0 \tag{26}$$

$$\eta = \pm \bar{l}_y: \quad g = h = 0, \quad \frac{\partial f}{\partial \xi} + \frac{\partial h}{\partial \eta} = 0 \quad \times\left(\bar{l}_x = l_x / t, l_y = l_y / t\right). \tag{27}$$

Let us choose the finite difference rectangular grid with grid cell size, $\Delta\xi$ and $\Delta\eta$, measured in whole numbers. Designate:

$$f_{m,n} = f(m,n), \quad g_{m,n} = g(m,n), \quad h_{m,n} = h(m,n). \tag{28}$$

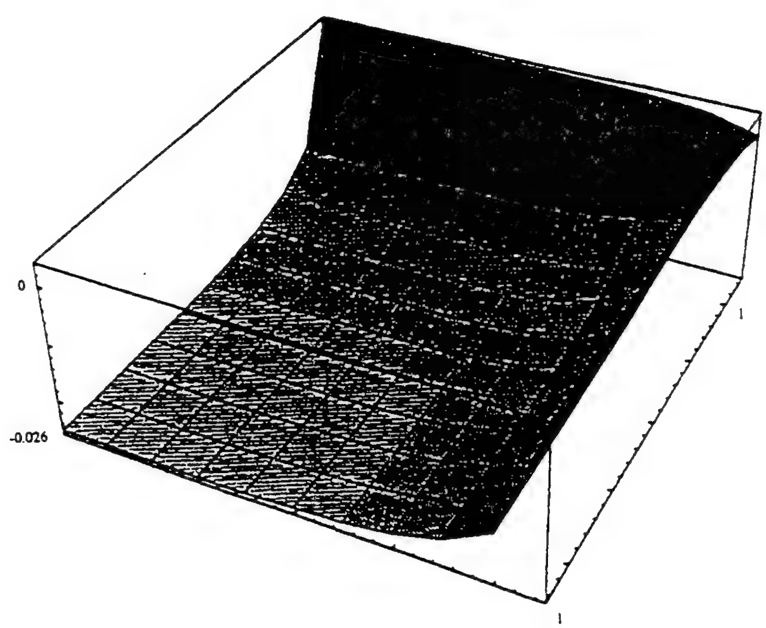


FIG. 2 The 3-D graphics of the sum $\sigma_x + \sigma_y$, in terms of $\bar{x}$ and $\bar{y}$.

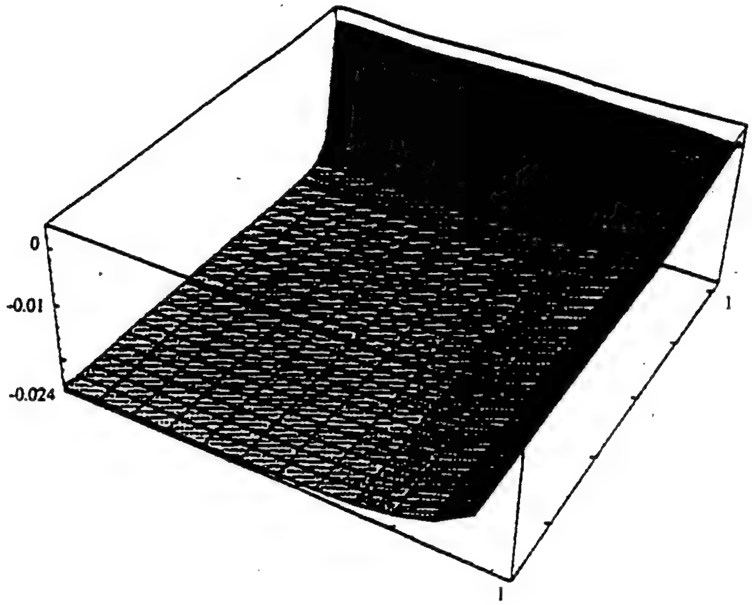


FIG. 3. The maximum shear stress $|\sigma_y - \sigma_x + 2i\tau_{xy}|/2$, in terms of $\bar{x}$ and $\bar{y}$.

The value of $\Delta\xi$ and $\Delta\eta$ less than 1 has no meaning, because the governing equation system (14)-(16) loses sense when the characteristic size of a domain in the xy plane has an order of the film thickness.

In the finite difference form the equation system (14)-(16), by taking $\Delta\xi = 1$ and $\Delta\eta = 1$, can be written as follows:

$$f_{m+1.n} - 2f_{m.n} + f_{m-1.n} + h_{m.n} + \frac{1}{2}h_{m+1.n-1} + \frac{1}{2}h_{m-1.n-1} - \frac{1}{2}h_{m+1.n} - \frac{1}{2}h_{m-1.n} - \frac{1}{2}h_{m.n+1}$$
$$-\frac{1}{2}h_{m.n-1} = \lambda\left(f_{m.n} - \nu_f g_{\mathrm{m.n}} + a\right); \tag{29}$$

$$g_{m.n+1} - 2gm.n + g_{m.n-1} + h_{m.n} + \frac{1}{2}h_{m+1.n+1} + \frac{1}{2}h_{m-1.n-1} - \frac{1}{2}h_{m+1.n} - \frac{1}{2}h_{m-1.n}$$
$$-\frac{1}{2}h_{m.n+1} - \frac{1}{2}h_{m.n-1} = \lambda\left(g_{m.n} - \nu_f f_{m.n} + b\right) \quad . \tag{30}$$

$$(f+g)_{m.n} + \frac{1}{2}(f+g)_{m+1.n+1} + \frac{1}{2}(f+g)_{m-1.n-1} - \frac{1}{2}(f+g)_{m+1.n} - \frac{1}{2}(f+g)_{m-1.n}$$
$$-\frac{1}{2}(f+g)_{m,n+1} - \frac{1}{2}(f+g)_{m.n-1} + h_{m+1.n} - 2h_{m.n} + h_{m-1.n} + h_{m.n+1} - 2h_{m.n}$$
$$+ h_{m.n-1} = \lambda\left[2(1+\nu_f)h_{m.n} - c\right].$$

(31)

The boundary condition equations, (26) and (27), are:

$$m = M: \quad f_{Mn} = h_{Mn} = 0, \; g_{m.n+1} - g_{M.n} = h_{M\text{-}1.n} - h_{M.n} \tag{32}$$

$$n = N: \quad g_{mN} = h_{mN} = 0, \quad f_{m+1.N} - f_{mN} = -h_{mN} + h_{mN-1} \; . \tag{33}$$

4. NUMERICAL EXAMPLE

To examine the numerical model (29)-(33) let us consider the normal isothermal expansion with no additional loadings. In this case:

$$a = b(\alpha_f - \alpha_s)\Delta T, \quad c = 0 \quad . \tag{34}$$

Consider the following data:

silicon substrate (Si)

$\alpha_s = 2.6 \times 10^{-6°}C; \quad v_s = 0.27; \quad G_s = 105$ Gpa;

lead thin film (Pb)

$\alpha_f = 29.5 \times 10^{-6°}C; \quad v_r = 0.37; \quad E_f = 80$ Gpa;

film geometry (25 × 100 rectangular domain)

$\bar{l}_x = M = 12; \quad \bar{l}_y = N = 50; \quad t = 1 \quad \mu m; \quad t_b = 3 \quad \mu m;$

The temperature difference, from manufacturing to operation, is

$$\Delta T = 300°C$$

Hence, we have

$$\lambda = \frac{tG_s}{t_b E_f} = 0.625, \quad a = b = 8 \times 10^{-3},$$
$$c = 0 \quad v_f = 0.37.$$

The authors did not have available detailed data on the variation of thermal expansion and elastic constants with temperature in this range, therefore, the material parameters were taken invariable in the present numerical example.

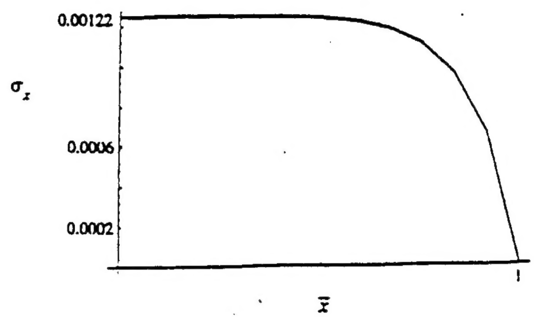


FIG. 4. Stress σ_x vs. $\bar{x}$ for $\bar{y}$ = 1, 0 < $\bar{x}$ < 1.

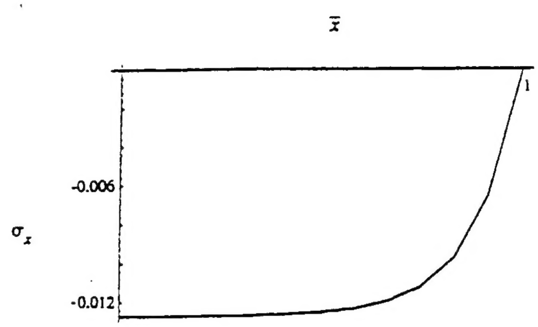


FIG. 5. Stress σ_x vs. $\bar{x}$ for $\bar{y}$ = 0, 0 < $\bar{x}$ < 1.

The calculation was done using *Matematica* and a finite difference model with grid 25 × 100. The results of the calculation are depicted on Figs. 2-7 for the quarter, $0 < x < a$ and $0 < y < b$, which is sufficient because of symmetry. The dimensionless values

$$\sigma_x - \frac{\Delta\bar{\sigma}_x}{E}, \quad \sigma_y = \frac{\Delta\bar{\sigma}_y}{E}, \quad \tau_{xy} = \frac{\Delta\bar{\tau}_{xy}}{E}, \qquad (35)$$
$$\bar{x} = \frac{x}{a}, \quad \bar{y} = \frac{y}{b},$$

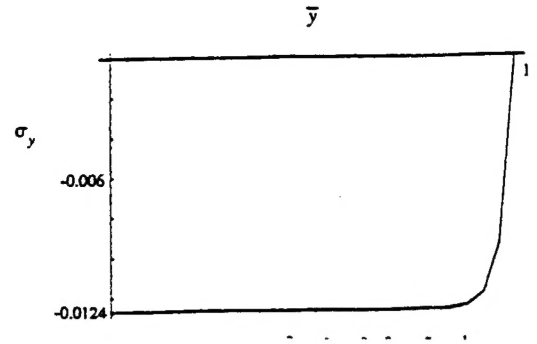


FIG. 6. Stress σ_y vs $\bar{y}$ for $\bar{x} = 0. 0 < \bar{y} < 1$.

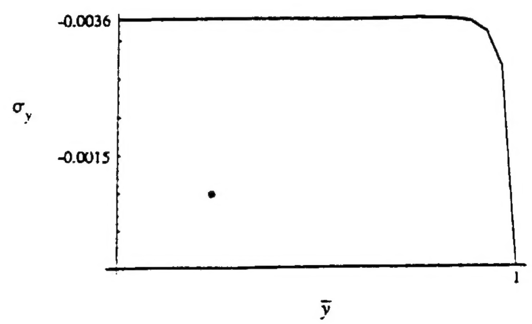


FIG. 7. Stress σ_x vs. $\bar{y}$ for $\bar{x} = 1, 0 < \bar{y} < 1$.

were used in Figs. 2-7.

Figures 2 and 3 show the three-dimensional graphics of the s um, $\sigma_x + \sigma_y$, and maximum shear stress in terms of $\bar{x}$ and $\bar{y}$. They demonstrate the uniform internal solution similar to a potential flow of an inviscid fluid and the boundary layer solution around the boundary of the rectangular domain. Figures 4-7 show the distribution of the characteristic non-zero stresses, σ_x and σ_y, along the boundary contour and the symmetry lines of the domain.

5. CONCLUSION TO PART 3

A numerical code was suggested to find thermal stresses in thin films and bonding layers. An examination of the model proved that a narrow boundary layer exists in the neighborhood of the border of the domain occupied by the thin film or bonding layers.

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